Nuclear structure from HF

Agenda:

1) How to include V_{3N}?
2) How to compute other observables?

⇒ Continue work on Exercise 2

3) Review main results
4) Orbital optimization in HF
5) Drip line of oxygen isotopes
6) Bigger code?

→ $e_{max} = 8$ possible

1) How to include V_{3N}?

V_{pqrstu} for basis of $N = 140$ states

$N^6 \sim 60$ TB

Why?

→ Not being clever with how we store things

- example, we store matrix elements $= 0$ that clearly violate symmetries

→ But V_{3N} is a hard problem!

- available for Hartree-Fock for nuclei since ~ 2010
- significant progress in 2020 - 2022
- still requires ~ 100 GB for large-scale calculations

Consider 3N contribution to E, F_{pq}:

$$E = \sum_{pq} \rho_{pq} H_{pq} + \frac{1}{2} \sum_{pqrs} \rho_{pq} \rho_{rs} H_{prqs} + \frac{1}{6} \sum_{pqrstu} \rho_{pq} \rho_{rs} \rho_{tu} V^{(3N)}_{prtqsu}$$

$$F_{pq} = H_{pq} + \sum_{rs} \rho_{rs} H_{prqs} + \frac{1}{2} \sum_{rstu} \rho_{rs} \rho_{tu} V^{(3N)}_{prtqsu}$$

Both equations depend on

$$H^{3B,\text{eff}}_{prqs} = \sum_{tu} \rho_{tu} V^{(3N)}_{prtqsu}$$

If we know ρ we can cheaply store effective two-body part of V^{3N}_{pqrstu}

Hebeler et al. Phys. Rev. C (2022)

Replace complicated equations with

$$E = \sum_{pq} P_{pq} H_{pq} + \frac{1}{2} \sum_{pqrs} P_{pq} P_{rs} H_{prqs} + \frac{1}{6} \sum_{pqrs} P_{pq} P_{rs} H^{3B,\text{eff.}}_{prqs}$$

$$F_{pq} = H_{pq} + \sum_{rs} P_{rs} H_{prqs} + \frac{1}{2} \sum_{rs} P_{rs} H^{3B,\text{eff.}}_{prqs}$$

same as normal 2B term but different factors

$\Rightarrow$ b/c actually 3B

How to solve HF with 3N interactions

- read in additional $H^{3B\,eff}_{pqrs}$
- implement new energy and Fock matrix functions

⇒ Done!

Questions?

Computing other observables

- ground state is easy

1) Identify associated operator $\hat{O}$ for observable O

example: $R_p^2 = \frac{1}{Z}\sum_{i=\text{proton}} r_i^2$ (point-proton radius squared!)

careful: 2-body correction required

2) evaluate expectation value like energy

$$\langle \hat{O} \rangle = \sum_{pq} P_{pq} O_{pq} + \frac{1}{2} \sum_{pqrs} P_{pq} P_{rs} O_{prqs}$$

- transitions and excited states are less clear
- can compute excited states from HF ground state, but these are not well optimized